Hartree-Fock Calculation for Finite Nuclei with a Nonlocal Two-Body Potential*†

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An application of the Hartree-Fock (HF) method to calculation of the structure of finite nuclei is presented. The nonlocal, separable potential of Tabakin is used as the two-body interaction. The calculation is carried out by writing the HF equations in an oscillator basis and applying the Moshinsky transformation to relative coordinates. The closed-shell nuclei O^{16} and Ca^{40} are considered. Under the assumption that they are spherical, their binding energy per particle is found to be -2.41 and -3.74 MeV for O^{16} and Ca^{40}, respectively. Possible reasons for the large discrepancy with the experimental binding are discussed. The single-particle energies show better agreement with data, but have too much spin-orbit splitting, namely, 10.2 MeV for $1p$ states in O^{16}, and 11.13 and 14.59 MeV, respectively, for the $1p$ and $1d$ states in Ca^{40}. The rms radii for O^{16} and Ca^{40} were found to be 2.38 and 2.96 F, compared with experimental values of 2.64 F and 3.52 F, respectively. Corrections for Coulomb force and center-of-mass motion have also been calculated.

INTRODUCTION

CALCULATIONS of the structure of finite nuclei from fundamental principles, until recently, have been complicated by the nature of the two-body interaction. In order to fit all the data, it was found that the local two-body interaction[1] must have a hard core; i.e., infinite repulsion inside some core radius. Because of this, the Hartree-Fock (HF) method,[2] which had proved so convenient in atomic physics, could not be used in nuclear-structure calculations. To deal with the hard cores, the much more difficult Brueckner theory[3] had to be applied. Finite-nucleus calculations with this theory have been done by Brueckner and co-workers,[4] but it is not clear whether the assumptions they make are valid. It would be better if a nonsingular two-body potential could be found so that the simpler HF method can be applied. Besides being simple, the HF method has been extended to correlated systems by means of the Bogoliubov-Valatin transformation and the random phase approximation. No such extensions exist for Brueckner theory.

The nonlocal potential of Tabakin[5] was designed to enable application of the Hartree-Fock method to calculations of the structure of finite nuclei. The present paper is a summary of the results of one such HF calculation[6] for the nuclei O^{16} and Ca^{40}. It is shown that qualitative agreement with experimental data is possible, but that severe discrepancies remain, notably in the total binding energy. This calculation is in many ways similar to a recent calculation of Muthukrishnan and Baranger,[7] but in our case the potential is one which fits all two-body data as well as nuclear matter, whereas that in Ref. 7 fits only nuclear matter. Our potential has the full complication of tensor and spin-orbit forces, but that in Ref. 7 is purely central, though also nonlocal. The results in both cases show similar trends and indicate the usefulness of the method used here.

I. METHOD OF CALCULATION

1. The Hartree-Fock Equations

The HF equations are solved by the matrix method[8] using a basis of harmonic-oscillator wave functions. The single-particle states ψ_α are expanded in a finite series of oscillator wave functions ϕ_μ:

$$\psi_\alpha(\mathbf{r})=\sum_\mu C_\mu{}^\alpha\phi_\mu(\mathbf{r}). \quad (1)$$

The expansion coefficients $C_\mu{}^\alpha$ as well as the number of terms N in the expansion and the oscillator parameter $\gamma=\hbar/(M\omega)$ are parameters to be determined by the HF procedure. The assumption of spherical nuclei is made. Then, ψ_α have good orbital and total angular momentum and the $C_\mu{}^\alpha$ are diagonal in angular momentum quantum numbers and are real. Hence, the sum in Eq. (1) is over the principal quantum number only. With this representation, the HF equations have the form of a set of finite matrix diagonalizations, one for each value of orbital and total angular momentum

$$\sum_{\mu'}\langle\mu|\,(t+U)\,|\mu'\rangle C_{\mu'}{}^\alpha=\epsilon_\alpha C_\mu{}^\alpha. \quad (2)$$

Here t is the kinetic energy operator $p^2/(2M)$ and U is the effective potential defined in terms of antisymmetrized matrix elements of the two-body interaction v by

$$\langle\mu|\,U\,|\mu'\rangle=\sum_{\nu\nu'}\rho_{\nu\nu'}\langle\mu\nu|\,v_A\,|\mu'\nu'\rangle, \quad (3)$$

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[1] T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 382 (1962).

[2] F. Villars, in *Proceedings of the International School of Physics "Enrico Fermi," Course 23*, edited by V. F. Weisskopf (Academic Press Inc., New York, 1963).

[3] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958).

[4] K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. **121**, 255 (1961), here referred to as BLR: K. S. Masterson, Jr., and A. M. Lockett, *ibid.* **129**, 776 (1963).

[5] F. Tabakin, Ann. Phys. (N.Y.) **30**, 51 (1964); Ph.D. thesis, MIT, 1963 (unpublished).

[6] J. P. Svenne, Ph.D. thesis, MIT, 1965 (unpublished).

[7] R. Muthukrishnan and M. Baranger, Phys. Letters **18**, 160 (1965).

[8] M. Baranger, *Cargèse Lectures in Theoretical Physics* (W. A. Benjamin, Inc., New York, 1963); R. K. Nesbet, Rev. Mod. Phys. **35**, 552 (1963).

where $\rho_{\mu\mu'}$ is the density matrix, defined as

$$\rho_{\mu\mu'}=\sum_\alpha C_\mu{}^\alpha C_{\mu'}{}^\alpha. \quad (4)$$

The summation is over occupied states only. Then, the total binding energy is

$$E_0=\sum_{\mu\mu'}\rho_{\mu\mu'}\langle\mu|(t+\tfrac{1}{2}U)|\mu'\rangle. \quad (5)$$

The detailed calculations are given in Ref. 6. The most difficult part of the calculation is the evaluation of the matrix elements of the two-body interaction in Eq. (3). Here, it is essential that the potential v be nonsingular, having no hard core, in order that the matrix element be finite. And it is here that the usefulness of the oscillator expansion is apparent. Because the states $|\mu\nu\rangle$ are oscillator states, it is possible to make the transformation to relative and center-of-mass coordinates, according to Brody and Moshinsky[9]:

$$|n_1l_1,n_2l_2;\lambda m_\lambda\rangle=\sum_{nlNL}|nl,NL;\lambda m_\lambda\rangle \times\langle nl,NL;\lambda|n_1l_1,n_2l_2;\lambda\rangle. \quad (6)$$

The state $|n_1l_1,n_2l_2;\lambda m_\lambda\rangle$ is the product state of particle 1 in an oscillator state with principal quantum number n_1, orbital angular momentum l_1, particle 2 in oscillator state n_2l_2 and the angular momenta coupled to λm_λ. The state $|nl,NL;\lambda m_\lambda\rangle$ has the relative coordinate in oscillator state nl, the center of mass in NL, and the angular momenta again coupled to λm_λ. The transformation brackets have a number of simple properties which are listed in Ref. 9 along with tables for $2n_1+l_1\leqslant 6$.

Corrections for the effects of the Coulomb potential and center-of-mass motion were computed. The Coulomb correction is included exactly by taking the total two-body interaction as Tabakin's plus the Coulomb potential, taking account of the fact that the Coulomb potential acts between protons only. The wave functions obtained with and without the Coulomb correction were not significantly different. Therefore, the total Coulomb energy could be taken as the difference in E_0 with and without the Coulomb force. The center-of-mass motion was considered by subtraction of the center-of-mass kinetic energy $P^2/(2MA)$ from the total Hamiltonian. This kinetic energy operator can be written as a sum of one-body and two-body operators. The two-body operator is usually written in the form

$$\sum_{i\neq j}\mathbf{p}_i\cdot\mathbf{p}_j,$$

but it may also be expressed in terms of the relative momentum $\mathbf{p}_{ij}=\frac{1}{2}(\mathbf{p}_i-\mathbf{p}_j)$, so that the Moshinsky transformation can be used. Then the one-body operator cancels exactly the one-body operator t in the total Hamiltonian. As a result, in Eqs. (2) and (5) the term in t is gone, but in Eq. (3), v has an additional term $2p_{ij}{}^2/(MA)$. Also, in Eq. (2) the eigenvalue is no longer the single-particle energy, but it is the single-particle energy plus the average kinetic energy. Thus, Eq. (2) is replaced by

$$\sum_{\mu'}\langle\mu|U|\mu'\rangle C_{\mu'}{}^\alpha=(\epsilon_\alpha+\bar{t})C_\mu{}^\alpha, \quad (7)$$

where $\bar{t}=\sum_{\mu\mu'}\rho_{\mu\mu'}\langle\mu|t|\mu'\rangle/A$. The expectation value of the center-of-mass kinetic energy $E_{\text{c.m.}}=\langle P^2/(2MA)\rangle$ can be taken approximately as the difference in E_0 with and without the center-of-mass correction, since the wave functions in the two cases do not differ significantly.

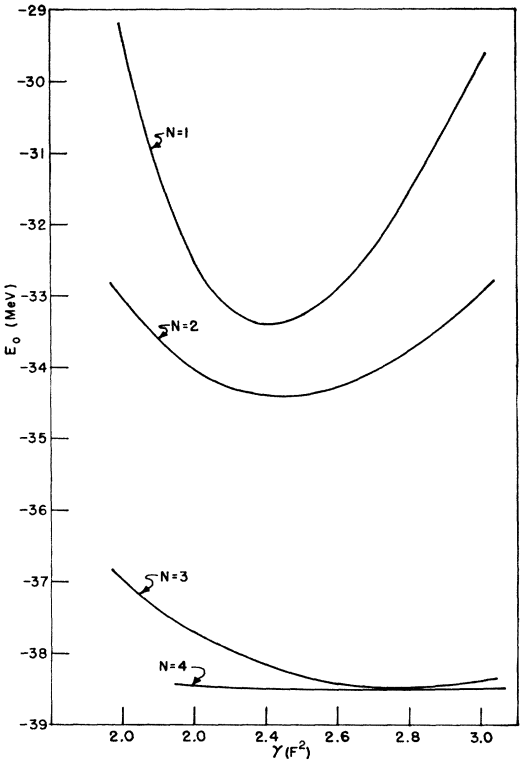

FIG. 1. Behavior of E_0 with γ and N for O^{16}.

2. The Two-Body Interaction

The Tabakin potential[5] has been used as the two-body interaction v. This is a nonlocal potential, written as a sum of separable terms containing parameters which have been determined by a fit to the two-body scattering and bound-state data. This potential is smooth, having none of the difficulties generated by the hard core in conventional local interactions. The energy per particle (E/A) in nuclear matter has been calculated in Ref. 5. The first-order E/A saturates at a minimum of -8 MeV at $k_F=1.6$ F^{-1}; with the second-order term included, E/A has a minimum of -14.1 MeV at $k_F=1.8$ F^{-1}. This is to be compared with the empirical values: $E/A=-15.75$ MeV, $k_F=1.5$ F^{-1}. One may expect this potential to be suitable for a HF calculation.

[9] T. A. Brody and M. Moshinsky, *Tables of Transformation Brackets* (Monografias del Instituto de Fisica, Mexico, 1960).

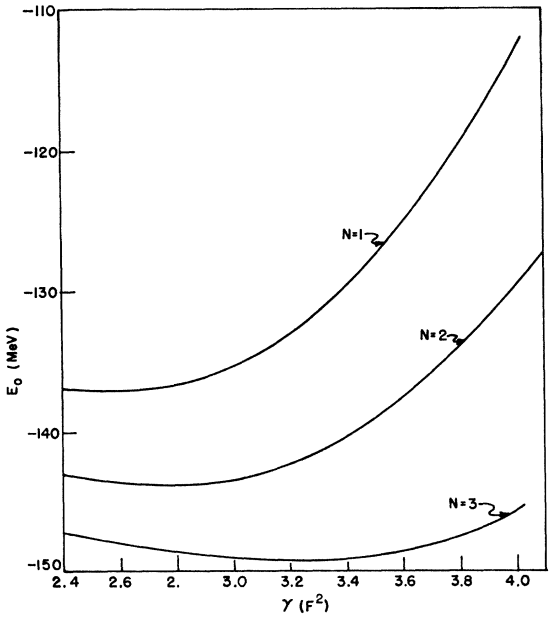

FIG. 2. Behavior of E_0 with γ and N for Ca^{40}.

3. Computation

The solution of Eq. (2) was done by computer using an iterative method. An initial set of expansion coefficients C_μ^α was chosen, the effective potential U was computed, using Eqs. (3) and (4) and the diagonalization (2) performed. This yielded a new set of coefficients C_μ^α which initiated the next cycle. At each stage E_0 was computed and the iteration was stopped when E_0 reached a constant value. This was done for a series of values of N and γ and the minimum in E_0 as a function of γ was found.

II. RESULTS

The result of this search, for O^{16}, is shown in Fig. 1. For $N=3$, the minimum is at $\gamma=2.8$ F^2, $E_0=-38.47$ MeV. A similar calculation (Fig. 2) for Ca^{40} yields a minimum at $\gamma=3.0$ F^2, $E_0=-149.69$ MeV. The sensitivity of E_0 to γ decreases as N increases. This is reasonable since for $N\rightarrow\infty$ the wave function ψ_α is represented exactly by the expansion (1) for all values of γ; hence, E_0 must be independent of γ in this limit. The complete results for E_0/A (A is the mass number) are given in Table I, and a comparison with calculations using hard-core potentials and Brueckner theory,[4] and perturbation theory with soft-core potentials,[10] and with experimental data[11] is shown.

Corrections due to the Coulomb force and center-of-mass motion were calculated. The Coulomb energy was $E_{\text{Coul}}=15.30$ MeV for O^{16} and 73.55 MeV for Ca^{40}. The usual formula $E_{\text{Coul}}=\frac{3}{5}e^2Z(Z-1)/R$ gives 14.77 and 73.84 MeV for O^{16} and Ca^{40}, respectively. The average

[10] P. Goldhammer, Phys. Rev. 116, 676 (1959).
[11] A. H. Wapstra, Physica 21, 367, 385 (1955).

TABLE I. Comparison of E_0/A (MeV/particle) for O^{16}, Ca^{40} with other calculations and data.

Nucleus		O^{16}	Ca^{40}
This work		−2.41	−3.74
BLR,[a] core contribution times α	$\alpha=1.0$	−2.02	−3.89
	$\alpha<1.0$	$(\alpha=0.825)-4.41$	$(\alpha=0.9)-6.12$
Masterson and Lockett[a]			−6.55
Goldhammer[b]		−8.07	
Data[c]		−7.98	−8.55

[a] Reference 4.
[b] Reference 10.
[c] Reference 11.

center-of-mass kinetic energy in the HF solution was $E_{\text{c.m.}}=\langle P^2/(2MA)\rangle=13.00$ MeV for O^{16} and 10.82 MeV for Ca^{40}. There is an accidental cancellation of Coulomb and center-of-mass corrections in the case of O^{16}.

The single-particle energies are the eigenvalues ϵ_α in Eq. (2). These are shown for O^{16} and Ca^{40} in Tables II and III. They are compared with Brueckner-theory calculations[4] and the experimental data from $(p,2p)$ experiments[12] and stripping reactions.[13] The single-particle levels obtained here compare well with the empirical values, but are more spread out, the high ones too high, the low ones too low. In particular, the spin-orbit splitting is too great. For O^{16}, the $1p_{1/2}-1p_{3/2}$ splitting is 10.2 MeV, compared to the empirical 6.16 MeV; for Ca^{40} the $1p_{1/2}-1p_{3/2}$ splitting is 11.13 MeV, the $1d_{3/2}-1d_{5/2}$ is 14.59 MeV, the empirical value for the d states being 7.0 MeV. In addition there is a large gap (11.76 MeV for O^{16}) between occupied and unoccupied levels. This is consistent with the observations of Kelson and Levinson[14] and is probably an important feature of HF calculations.

Also calculated were the single-particle wave functions, particle density, and rms radius. The detailed

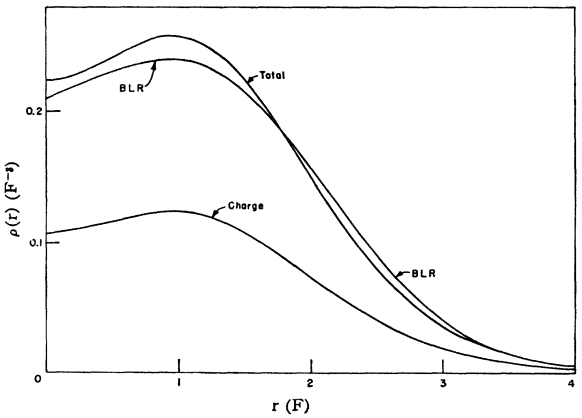

FIG. 3. Total and charge density in O^{16}.

[12] M. Riou, Rev. Mod. Phys. 37, 375 (1965).
[13] B. L. Cohen, Phys. Rev. 130, 227 (1963).
[14] I. Kelson and C. A. Levinson, Phys. Rev. 134, B269 (1964).

TABLE II. Single-particle energies in O^{16}, in MeV.

	This work ($\gamma=2.4$ F^2, $N=3$)						
	No c.m. correction		With c.m. correction	BLR[a]		Data	
State	Neutron	Proton	Neutron	Neutron	Proton	Neutron[b]	Proton[c]
$1s_{1/2}$	−48.72	−41.88	−50.55	−44.3	−39.6		−34±3.5
$1p_{3/2}$	−19.65	−14.71	−23.07	−19.0	−14.6	−21.81	−18±2.5
$1p_{1/2}$	−9.45	−5.83	−11.56	−14.9	−10.7	−15.65	−13±2
$1d_{5/2}$	2.31					−5.02	
$2s_{1/2}$	6.12	9.38	7.16			−4.15	
$1d_{3/2}$	10.74					0.93	

[a] Reference 4.
[b] Neutron energies are taken from Ref. 13.
[c] Proton energies are taken from Ref. 12.

TABLE III. Single-particle energies in Ca^{40}, in MeV.

	This work ($\gamma=3.0$ F^2, $N=3$)								
	No c.m. correction		With c.m. correction	BLR[a]		Masterson and Lockett[a]		Data	
State	Neutron	Proton	Neutron	Neutron	Proton	Neutron	Proton	Neutron[b]	Proton[c]
$1s_{1/2}$	−71.80	−62.35	−75.57	−70.1	−60.0	−48.7	−41.4		
$1p_{3/2}$	−44.87	−36.99	−47.40	−44.7	−35.1	−34.0	−26.7		
$1p_{1/2}$	−34.73	−26.88	−36.05	−38.6	−24.2	−30.4	−23.2		
$1d_{5/2}$	−20.99	−14.42	−23.31	−20.6	−11.6	−17.5	−10.3	−22.8	−14.5
$2s_{1/2}$	−14.13	−6.94	−15.38	−16.0	−7.3	−14.8	−7.6	−18.4	−10.6
$1d_{3/2}$	−7.66	−1.38	−8.23	−13.4	−4.9	−12.6	−5.5	−15.8	−8.3

[a] Reference 4.
[b] Neutron energies are taken from Ref. 13.
[c] Proton energies are taken from Ref. 12.

results of these calculations are given in Ref. 6. Table IV is a summary of the rms radius values and Figs. 3 and 4 show the total and charge density in O^{16} and Ca^{40} respectively. The total density is compared to that of BLR[4] obtained by Brueckner theory. The rms radii and densities are close to the experimental values and to what one expects from previous calculations with other potentials. The rms radii are too small, as in other calculations, but one might expect higher order effects to increase the radii, since these effects will bring in states with higher principal quantum number and longer range.

TABLE IV. Rms and charge radius (in F) for O^{16} and Ca^{40}; comparison with other calculations and data.

		Nucleus	
Source	Type	O^{16}	Ca^{40}
This work	Charge	2.420	2.992
	Total	2.380	2.963
This work with c.m. correction	Total	2.276	2.870
BLR[a]	Charge	2.41	2.91
	Total	2.40	2.88
Masterson and Lockett[a]	Charge		3.00
	Total		2.99
Goldhammer[b]	Total	2.33	
Data[c]	Charge	2.64	3.52

[a] Reference 4.
[b] Reference 10.
[c] R. Hofstadter, Ann. Rev. Nucl. Sci. **7**, 231 (1959).

III. CONCLUSIONS

It has been demonstrated that the HF method in an oscillator basis is applicable to calculation of the structure of finite nuclei if a nonsingular two-body force is available. The results of such a calculation are, on the whole, very good. The radius and density, the single-particle energies, the Coulomb energy compare well with

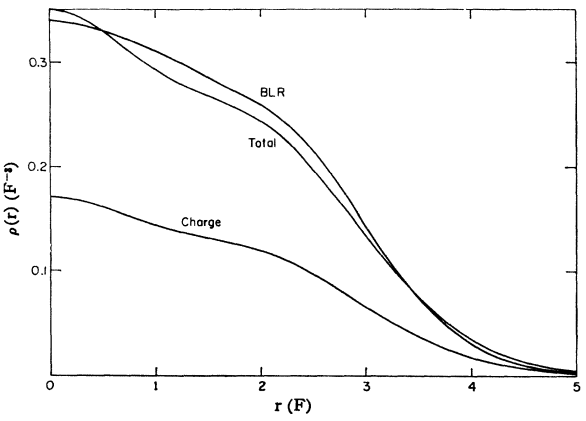

FIG. 4. Total and charge density in Ca^{40}.

what is expected from other calculations and experimental evidence. The oscillator expansion (1) converges very rapidly, 3–4 terms being quite sufficient. This agrees with the observation of Muthukrishnan and Baranger[7] who find four terms sufficient for the single-particle energies. To find the wave functions correctly, Davies *et al.*[15] need eight or more terms. This is necessary to give these functions the proper exponential behavior at large r, but these higher terms have little effect on the energies.

However, the large discrepancies in E_0/A and the spin-orbit splitting are disturbing, and an explanation is needed. A large part of the error can possibly be attributed to the Tabakin potential, since it does not fit the data too well. A similar calculation with a more realistic potential is not yet available for comparison.[16] The potential used in Ref. 7 is a much cruder fit to the data. It does not seem likely that the additional binding needed can be obtained by taking more terms in the oscillator series. The convergence of the series is so good that higher terms cannot be expected to give the additional 5.57-MeV/particle binding required in O^{16}. Since the HF equations come from a variational principle, any relaxation of the constraints imposed on the ψ_α by the assumption of spherical nuclei and good parity could increase the binding (make E_0 more negative).[17] Whether this will be sufficient cannot be estimated at this time.

The importance of second-order effects should also be considered. In the nuclear matter calculation, Tabakin[5] found a second-order potential energy of $V^{(2)}=-6$ MeV/particle. The first-order potential energy was $V^{(1)}=-40$ MeV/particle. If we assume this ratio $V^{(2)}/V^{(1)}=0.15$ to hold in the finite nuclei, we can estimate the second-order effect for this case. Such an assumption is not unreasonable since the second-order calculation involves excitation to high energy states whose wave functions are approximately plane waves. Hence, the same type of matrix elements enter in the nuclear matter calculation. In O^{16} we obtained a first-order potential energy of $V^{(1)}=-351$ MeV. Then $V^{(2)}=0.15V^{(1)}=-53$ MeV. Adding this to the total energy obtained for O^{16}, we get $E_0{}^{(2)}=-91$ MeV. This compares much better with the experimental number of -127.7 MeV. A similar calculation for Ca^{40} gives $V^{(2)}=-157$ MeV, then $E_0{}^{(2)}=-307$ MeV. This experimental value is -324.1 MeV. Thus it is possible that all the required binding can be given by the higher order effects with good convergence.

The large spin-orbit splitting, likewise, may be attributed to the Tabakin potential until calculations with other potentials are available. There is no spin-orbit splitting in the calculation of Ref. 7. The Tabakin potential does not separate uniquely into central, tensor, and spin-orbit terms. Therefore, it is not possible to investigate the source of the large splitting. However, we have found that the $p_{1/2}$ and $p_{3/2}$ wave functions differ significantly, suggesting that the tensor force contributes to the spin-orbit splitting.

[15] K. T. R. Davies, S. J. Krieger, and M. Baranger, Nucl. Phys. (to be published).

[16] A calculation for O^{16} with the BKL potential [C. Bressel, A. Kerman, and E. Lomon, Bull. Am. Phys. Soc. 10, 584 (1965)] was attempted, but the core repulsion was still too strong and the system did not bind. However, when the Tabakin potential was allowed to act in the s states and the BKL in all other states, O^{16} did bind, but not as strongly as with pure Tabakin potential. This suggested that the core repulsion of the BKL potential could be reduced by making the core nonlocal. This program is currently being undertaken at this laboratory and there is hope that a realistic, nonsingular potential will soon be available which will be suitable for HF calculations.

[17] Work has recently been started to extend this HF calculation to deformed nuclei by mixing different orbital and total angular momenta in the sum in Eq. (1).